Understanding the properties of solid-liquid interfaces in terms of water structure at the various surfaces

Title of the dissertation
Structural and dynamic properties of the solid-liquid interfaces studied by Molecular Dynamics simulations

Contents of the dissertation
The experiments performed at solid-liquid interfaces are based on imaging the system with atomic resolution using atomic force microscopy (AFM). Although these images provide us with the structure of the hydration layers with molecular resolution, it is not always easy to understand the real physical processes at the interfaces. This is especially emphasised in the case of highly reactive step edges. In order to provide a better understanding of the processes being investigated by AFM, the system of interest is modelled at the molecular level and the theoretical simulations are performed under the exact same conditions, reproducing the real experiment. These simulations provide us with the new insights into the mechanism of the processes at the interfaces that can then help us to understand the nature of AFM images.

In this study, we apply such technique to study clay minerals in water, especially at the step edges that are responsible for dissolution and crystal growth. Apart from the hydration layers at the step edges, we also used simulation technique in order to study the influence of ions at the various solid-liquid interfaces and hence try to better understand the role ions play in high-resolution AFM imaging in liquids.

The method presented in the dissertation can in principle be applied to any system of interest as a support tool to AFM study. This way, it will provide a practical understanding and strong link between the systems prepared in the experimental work and real performance.

Field of the dissertation
Engineering Physics

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